Resonances in one-dimensional Disordered Chain

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Abstract

We study the average density of resonances, $\langle \rho(x,y) \rangle$, in a semi-infinite disordered chain coupled to a perfect lead. The function $\langle \rho(x,y) \rangle$ is defined in the complex energy plane and the distance y from the real axes determines the resonance width. We concentrate on strong disorder and derive the asymptotic behavior of $\langle \rho(x,y) \rangle$ in the limit of small y.

1 Introduction

Open quantum systems often exhibit the phenomenon of resonances. Resonances correspond to quasi-stationary states which have a long life-time but eventually decay into the continuum. (A particle, initially within the system, escapes to infinity.) They are characterized by complex energies, $\tilde{E}_\alpha = E_\alpha - \frac{i}{2}\Gamma_\alpha$, which correspond to poles of the S-matrix on the unphysical sheet of the complex energy plane [1, 2]. There are many examples of resonances in atomic and nuclear physics. More recently, there has been much interest in resonant phenomena in the field of chaotic and disordered systems (for recent reviews see [3, 4]).

There is considerable amount of work concerning the distribution $P(\Gamma)$ of resonance widths in one-dimensional disordered chains [5, 6, 7, 8, 9]. Numerical studies presented

in that work demonstrate that, in a broad range of Γ, $P(\Gamma) \propto \Gamma^{-\gamma}$, with the exponent γ being close to 1. (This behavior is not restricted to disordered chains, but pertains also to two- and three-dimensional systems with *localized* states [7, 9]). An intuitive argument, which assumes a uniform distribution for the localization centers of exponentially localized states, leads to a $(1/\Gamma)$-behavior [7, 8, 9]. The analytical calculation in [8], performed for a one-dimensional continuous (white-noise) potential, exhibits this behavior for sufficiently small Γ, followed by a sharp cutoff at still smaller Γ, due to the finite size of the sample. It is also shown in [8] that in a broad range of Γ, $P(\Gamma)$ is well fitted by a function $\Gamma^{-1.25}$. In the present Letter we develop an analytical approach for a discrete, tight-binding random chain. We treat the problem in the limit of *strong* disorder and derive the asymptotically exact $(1/\Gamma)$-behavior for a *semi-infinite* system.

2 The model and its Effective Hamiltonian

We consider a semi-infinite disordered chain coupled to a (semi-infinite) perfect lead. $n = 1, 2, ...$, designate sites along the chain. Each site of the chain is assigned a site energy, ϵ_n. Different ϵ_n's ($n = 1, 2, ...$) are independent random variables chosen from some symmetric distribution $q(\epsilon)$. Sites of the lead are labelled by $n = 0, -1, -2, ...$ All sites of the lead are assigned $\epsilon_n = 0$. The lead simulates the free space outside the chain. All nearest neighbor sites of the full system (chain + lead) are coupled to each other by a hopping amplitude t, so that a particle, initially located somewhere within the chain, will eventually escape into the lead.

The most direct approach to the problem of resonances amounts to solving the stationary Schrödinger equation, for the entire system, with the boundary condition of an *outgoing wave* only. This condition, which makes the problem non-Hermitian, describes a particle ejected from the system. The Schrödinger equation with such boundary condition admits complex eigenvalues $\tilde{E}_\alpha$, which correspond to the resonances [1, 2]. This kind of approach, which leads in a natural way to a non-Hermitian effective Hamiltonian, has been used for a long time in scattering theory, including scattering in chaotic and disordered systems ([4, 10], and references therein). For our system the approach amounts to solving the infinite set of coupled equations

$$-t\psi_{n+1} - t\psi_{n-1} + \epsilon_n\psi_n = \tilde{E}\psi_n \qquad (-\infty < n < \infty) \tag{1}$$

We recall that $\epsilon_n = 0$ for $n < 1$ (the lead) and it is random for $n \geq 1$ (the chain). Eqs.(1) are to be solved subjected to the boundary condition $\psi_n \propto \exp{-i\tilde{k}n}$, corresponding to an outgoing wave in the lead. The complex wave vector $\tilde{k}$ determines $\tilde{E}$ according to $\tilde{E} = -2t\cos\tilde{k}$. It is straightforward to eliminate from Eqs.(1) all ψ_n's with $n < 1$, thus reducing the problem to a system of equations for the amplitudes ψ_n on the sites of the disordered chain alone ($n = 1, 2, ...$).

$$-t\psi_{n+1} - t\psi_{n-1} + \tilde{\epsilon}_n\psi_n = \tilde{E}\psi_n \qquad (n = 1, 2, ...) \tag{2}$$

with the condition $\psi_0 = 0$. Here $\tilde{\epsilon}_n = \epsilon_n$ for $n = 2, 3, ...$, but not for $n = 1$. This end site is assigned a complex energy $\tilde{\epsilon}_1 = \epsilon_1 - t \exp i\tilde{k}$ which describes coupling to the outside world. Thus, the resonances are given by the complex eigenvalues of the non-Hermitian effective Hamiltonian defined in (2). Note that Eq. (2) does not constitute a standard eigenvalue problem because $\tilde{\epsilon}_1$ contains $\tilde{k}$, which is related to $\tilde{E}$. The problem is often simplified by fixing $\tilde{k}$ at some real value, consistent with the value of energy near which one is looking for resonances. Such simplification corresponds to replacing the "exact resonances" by "parametric" ones [5]. There are indications that for sufficiently narrow resonances the "parametric" and the "exact" distributions are close to one another. In this Letter we restrict ourselves to "parametric" resonances. For instance, close to the middle of the energy band we set $\tilde{k} = \pi/2$, thus arriving at the effective Hamiltonian

$$(H_{eff})_{nm} = \tilde{\epsilon}_n \delta_{nm} - t_{nm} \qquad (n = 1, 2, \ldots). \tag{3}$$

where $t_{nm} = t$ for nearest neighbors (and zero otherwise), and $\tilde{\epsilon}_1 = \epsilon_1 - it$. Let us repeat that all site energies, except for $\tilde{\epsilon}_1$, are real. The imaginary part $-it$ of $\tilde{\epsilon}_1$ accounts for the coupling of the chain to the lead, via the hopping amplitude t connecting site 1 to site 0. It is convenient to slightly generalize the model by assigning to this particular amplitude a value t', which can differ from all the other hopping amplitudes t. This allows us to tune the coupling from $t' = 0$ (closed chain) to $t' = t$ (fully coupled chain). In what follows we set $t = 1$ and denote the dimensionless coupling strength $v \equiv t'/t$.

3   The Average Density of Resonances

Resonances correspond to complex eigenvalues of H_{eff}, i.e., to the poles of the resolvent

$$\tilde{\mathbf{G}} = \frac{1}{z - H_{eff}} \tag{4}$$

in the lower half of the complex energy plane. We denote these poles by $z_\alpha = x_\alpha + iy_\alpha$. (These are just the complex energies $\tilde{E}_\alpha = E_\alpha - \frac{i}{2}\Gamma_\alpha$, of Section 1, in units of t which we set to 1.) The average density of these poles is defined as

$$\langle \rho(x, y) \rangle = \langle \sum_\alpha \delta(x - x_\alpha)\delta(y - y_\alpha) \rangle, \tag{5}$$

where $\langle \cdots \rangle$ denotes disorder averaging, i.e., averaging over all realizations of the set $\{\epsilon_n\}$ of the random site energies.

In order to appreciate the difference between $\langle \rho(x, y) \rangle$ and the probability distribution, $P(x, y)$, of resonance width y (for some fixed x) let us consider for a moment a finite chain, of N sites. In this case $P(x, y)$, by definition, is equal to $\langle \rho(x, y) \rangle$ divided by N. When N increases, $P(x, y)$ "runs away" towards smaller and smaller y's, and in the $N \to \infty$ limit it approaches $\delta(y)$. (Indeed, for a semi-infinite chain an eigenstate will be localized, with

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probability 1, at infinite distance from the open end and, thus, will be ignorant about the coupling to the external world.) On the other hand, $\langle\rho(x,y)\rangle$ does have a well defined $N \to \infty$ limit, for any fixed (non-zero) y. To clarify this assertion, we begin with a closed semi-infinite chain ($v = 0$). In this case all states are localized ($y_\alpha = 0$)- some close to the end (site 1)and some further away. When the chain is opened ($v = 1$), localized states turn into resonances. The point is that for fixed y (and x) the main contribution to $\langle\rho(x,y)\rangle$ will come from states that (for $v = 0$) were localized around some optimal distance $d(x,y)$ from the open end. Therefore distant pieces of the chain do not contribute to $\langle\rho(x,y)\rangle$ and a well defined $N \to \infty$ limit exists. The N necessary for achieving this limit will, of course, depend on y (and x) but the limit will eventually be achieved for any y, however small (different from zero). Thus, although for any finite N, $P(x,y)$ and $\langle\rho(x,y)\rangle$ differ only by the normalization factor N, it is $\langle\rho(x,y)\rangle$ that has a meaningful $N \to \infty$ limit. $\langle\rho(x,y)\rangle$ may be expressed in terms of the resolvent $\tilde{\mathbf{G}}$ as [11, 12]

$$\langle\rho(x,y)\rangle = \frac{1}{2\pi} \left(\partial_x + i\partial_y\right) \langle\mathrm{Tr}\tilde{\mathbf{G}}(x,y)\rangle . \tag{6}$$

One can interpret the z_α's as the positions of unit electric point charges in the plane, which give rise to an electric field $\mathbf{E} = E_x\hat{\mathbf{x}} + E_y\hat{\mathbf{y}}$. In this picture, one has simply $\mathrm{Tr}\tilde{\mathbf{G}}(x,y) = E_x - iE_y$, and (6) is then interpreted as the Poisson equation for the averaged electric field and charge density. Equation (6) holds also for a closed chain, if $\tilde{\mathbf{G}}(x,y)$ is replaced by $\mathbf{G}(x,y)$, where the untilded $\mathbf{G}$ is the resolvent of the Hermitian Hamiltonian of the closed chain. In this case all the charges must lie on the real axis. Therefore, for any y different from zero, one can rewrite (6) as

$$\langle\rho(x,y)\rangle = \frac{1}{2\pi} \left(\partial_x + i\partial_y\right) \langle\mathrm{Tr}(\tilde{\mathbf{G}} - \mathbf{G})\rangle . \tag{7}$$

The advantage of this representation is that, although both $\mathrm{Tr}\tilde{\mathbf{G}}$ and $\mathrm{Tr}\mathbf{G}$ diverge in the $N \to \infty$ limit, $\mathrm{Tr}(\tilde{\mathbf{G}} - \mathbf{G})$ remains finite. (Of course, it is still perfectly all right to use (6), with the proviso that the derivative with respect to y is taken before taking the $N \to \infty$ limit.)

The electrostatic analogy just mentioned makes it clear that $\langle\mathrm{Tr}\tilde{\mathbf{G}}(x,y)\rangle$ cannot be a complex analytic function of $z = x + iy$, but must depend separately on x and y. This lack of analyticity makes the computation of $\langle\rho(x,y)\rangle$ a more difficult task than that of the density of states for a closed (Hermitian) system. In the latter case there is a well known representation of the resolvent

$$\mathbf{G_{nn}}(z) = \frac{1}{z - \epsilon_n - \Sigma_n(z)} . \tag{8}$$

where $\Sigma_n(z)$ is the self-energy at site n. Let us stress that (8) applies to a specific realization of random site energies $\{\epsilon_n\}$, i.e., $\Sigma_n(z)$ is a random quantity which depends on the set $\{\epsilon_n\}$. The statistical treatment of $\Sigma_n(z)$ forms the basis of many studies of the

localization problem [13], starting with the original work of Anderson [14]. The notion of self-energy can be generalized to our non-Hermitian problem, and the analog of (8) is

$$\tilde{\mathbf{G}}_{nn}(z) = \frac{1}{z - \epsilon_n - \tilde{\Sigma}_n(z)} \, . \tag{9}$$

This equation is essentially a definition of $\tilde{\Sigma}_n(z)$. It is convenient to assign the imaginary term $-iv$ to $\tilde{\Sigma}_1(z)$ rather than to the "bare" energy of the first site, so that all site energies, $\{\epsilon_n\}$, in (9) are real and are the same as for the corresponding closed chain. The term $-iv$ will appear as a boundary condition for the self energy and will play a crucial role, as demonstrated below.

In terms of the locator expansion [13, 14] $\tilde{\Sigma}_n(z)$ can be represented as a sum of paths which start at site n, visit other sites and then return (only once!) to the starting point n. Since the paths consist of steps connecting nearest neighbors (to the left or to the right), it is clear that $\tilde{\Sigma}_n(z)$ can be decomposed into two pieces, "left" and "right":

$$\tilde{\Sigma}_n(z) = \tilde{L}_n(z) + R_n(z) \tag{10}$$

The "left" self-energy, $\tilde{L}_n(z)$, depends only on the energies of sites to the left of site n, i.e., on ϵ_j's with $1 \leq j < n$. Similarly, R_n depends only on ϵ_j's with $j > n$ and, thus, it is ignorant about the fact that the chain is coupled to the outside world, via site 1 (that is why the R_n are not tilded). The reason for decomposing $\tilde{\Sigma}_n(z)$ into $\tilde{L}_n(z)$ and R_n is that these quantities obey simple recursion relations, which can be iterated to obtain their probability distributions:

$$\tilde{L}_j(z) = [z - \epsilon_{j-1} - \tilde{L}_{j-1}(z)]^{-1} \tag{11}$$

and

$$R_j(z) = [z - \epsilon_{j+1} - R_{j+1}(z)]^{-1} \tag{12}$$

Relation (11) has to be iterated starting with $j = 2$, with the "initial condition" $\tilde{L}_1 = -iv$. Relation (12), for the semi-infinite chain considered in this paper, leads to a stationary, n-independent distribution for the variable R_n. We will not need this distribution in the forthcoming calculation, restricted to the case of strong disorder.

4   Strong Disorder

Strong disorder means that a typical value of ϵ_n is much larger than $t = 1$, i.e., the distribution of site energies, $q(\epsilon)$, is very broad. In this case the above recursion relations simplify considerably. The real part of the self-energy can be neglected in comparison with ϵ_n, so that at any site n the real part of the resolvent is $Re\tilde{\mathbf{G}}_{nn}(z) \approx (x - \epsilon_n)^{-1}$,

which is the same as for the closed chain. Thus, the real parts of the two resolvents in (7) cancel out and one obtains

$$\langle \rho(x,y) \rangle = -\frac{1}{2\pi} \partial_y \langle \mathrm{Tr} Im(\tilde{\mathbf{G}} - \mathbf{G}) \rangle. \tag{13}$$

Furthermore, $Im\tilde{\mathbf{G}}_{nn}$ (see (9)) is dominated by $Im\tilde{L}_n(z)$ and can be approximated as

$$Im\tilde{\mathbf{G}}_{nn} = \frac{I_n - y}{(x - \epsilon_n)^2 + (I_n - y)^2} \approx \pi\delta(x - \epsilon_n)sign(I_n - y) \tag{14}$$

where, in order to avoid cluttering the notations, we denote $Im\tilde{L}_n(z) \equiv I_n$. Since ϵ_n and I_n are independent random variables, the averaging of (14) is done in two steps: first over ϵ_n, which gives the strong disorder limit of the density of states, $q(x)$, and then over I_n, with the yet unknown distribution $\tilde{P}_n(I)$. The latter is governed by the recursion relation (11), which in the strong disorder limit simplifies to

$$I_j = \frac{I_{j-1}}{(x - \epsilon_{j-1})^2}. \tag{15}$$

This equation, as well as the previous one, applies for $n \geq 2$. Site $n = 1$ provides the initial condition $I_1 = -v$. The recursion relation (15) "propagates" the information from the open end of the chain (site 1) to distant sites. Site 1 is special and should be excluded from the trace in (13). This is because I_1 has a fixed value, different from y. Using the electrostatic analogy, one can say that a charge, located away from the point (x,y) cannot produce a singularity at this point . Actually, (15) is valid only up to a point when I becomes of order y (recall that we are interested in y fixed but arbitrarily small, i.e., in the "small-y" asymptotic behavior of $\langle \rho(x,y) \rangle$). When such a small value of I is reached, the initial condition, i.e., the value of v, is forgotten, and there is no contribution to $\langle \rho(x,y) \rangle$ (more precisely, both $Im\tilde{\mathbf{G}}$ and $Im\mathbf{G}$ become very small and, moreover, cancel each other). In summary, averaging (14) with the distribution $\tilde{P}_n(I)$ and taking the derivative with respect to y, one obtains from (13) (with the $\mathbf{G}$-term neglected):

$$\langle \rho(x,y) \rangle = q(x) \sum_{n=2}^{\infty} \tilde{P}_n(y). \tag{16}$$

Eq. (16), supplemented by the recursion relation (15), enables us to obtain the asymptotic $(1/y)$-behavior, as we now explain. Note that the random variables I_n are negative, so that resonances are located in the lower half-plane of the complex variable z. It is more convenient to work with the absolute value, $|I_n|$, and to define y as positive, i.e., $\langle \rho(x,y) \rangle$ is the average density of resonances with width y (at energy x). Defining, instead of $|I_n|$, a new variable, $t_n = ln|I_n|$, and designating its distribution as $W_n(t)$, we have, instead of (16),

$$\langle \rho(0,y) \rangle = q(0)\frac{1}{y} \sum_{n=2}^{\infty} W_n(t), \qquad t = lny, \tag{17}$$

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where we set $x = 0$ (middle of the band). It follows from (15) and the initial condition $|I_1| = v = 1$ that

$$t_n = -2 \sum_{j=1}^{n-1} ln|\epsilon_j|, \tag{18}$$

so that

$$W_n(t) = < \int_{c-i\infty}^{c+i\infty} \frac{dp}{2\pi i} e^{p(t-t_n)} > = \int_{c-i\infty}^{c+i\infty} \frac{dp}{2\pi i} e^{pt} \nu^{j-1}(p), \tag{19}$$

where c is some real number and

$$\nu(p) = \int d\epsilon q(\epsilon) e^{2p ln|\epsilon|}. \tag{20}$$

Summing the geometric series in (17) we obtain:

$$\langle \rho(0, y) \rangle = q(0) \frac{1}{y} \int_{c-i\infty}^{c+i\infty} \frac{dp}{2\pi i} e^{pt} \frac{\nu(p)}{1 - \nu(p)}, \qquad t = lny. \tag{21}$$

This equation makes sense if $|\nu(p)| < 1$. A sufficient condition for this inequality is that c be negative and small, so that we have to choose the contour somewhat to the left of the imaginary axis in the complex p plane. In order to prove the $(1/y)$-behavior, in the small y limit, we have to verify that the integral in (21) approaches a constant (non-zero) value for $t \to -\infty$. It is intuitively quite obvious that in this limit, and for $|c| \ll 1$, the integral will be dominated by the vicinity of the point $p = 0$, near which $\nu(p) \approx 1 + 2p < ln |\epsilon| >$. For strong disorder, $< ln |\epsilon| >$ is positive and equal to the inverse localization length $1/\xi$ (in the middle of the band). Replacing in (21) $(1 - \nu(p))$ by $(-2p/\xi)$, we obtain:

$$\langle \rho(0, y) \rangle = q(0) \frac{1}{y} \int_{c-i\infty}^{c+i\infty} \frac{dp}{2\pi i} e^{pt} \frac{\nu(p)}{(-2p/\xi)} = \frac{q(0)\xi}{2y}. \tag{22}$$

Note that, since t is negative, the integration contour should be closed in the right half-plane, where Rep is positive, so that an extra minus sign is acquired. The formal proof of equivalence between (21) and (22), in the $t \to -\infty$ limit, is achieved by studying the difference between the two expressions. Let's denote by J and J' the integrals in (21) and (22), respectively. In both integrals c cannot be set equal to zero, because the integrand would diverge at $p = 0$. However, this divergence is cancelled in $J - J'$, so that for this quantity one can integrate directly along the imaginary p-axis. Moreover, since $\nu(p)$, for p purely imaginary, is just the characteristic function of the distribution for the variable $2ln|\epsilon|$, it must decrease faster than $1/|p|$ for large values of p. Therefore one can use the Riemann-Lebesgue lemma to prove that $J - J'$ approaches zero in the $t \to -\infty$ limit. This completes the proof of the main result, (22), of our paper. Equation (22), gives the

asymptotically exact expression for the average density of resonances in a semi-infinite, strongly disordered chain.

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